Toward the Ab-initio Description of Medium Mass Nuclei

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Abstract. As ab-initio calculations of atomic nuclei enter the A=40-100 mass range, a great challenge is how to approach the vast majority of open-shell (degenerate) isotopes. We add realistic three-nucleon interactions to the state of the art many-body Green's function theory of closed-shells, and find that physics of neutron driplines is reproduced with very good quality. Further, we introduce the Gorkov formalism to extend *ab-initio* theory to semi-magic, fully open-shell, isotopes. Proof-of-principle calculations for ^{44}Ca and ^{74}Ni confirm that this approach is indeed feasible. Combining these two advances (open-shells and three-nucleon interactions) requires longer, technical, work but it is otherwise within reach.

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Introduction. Microscopic first principle predictions of atomic nuclei are highly desirable since they can unambiguously guide research of exotic isotopes. These could also help in constraining extrapolations to higher mass regions [1] and to extreme proton-neutron asymmetries [2], including regions close to the driplines where experimental data is unlikely to become available in the foreseeable future.

Ab-initio methods such as coupled-cluster (CC) [3], in-medium similarity renormalization group (IMSRG) [4] or Dyson self-consistent Green's function [5, 6] (Dyson-SCGF) have accessed medium-mass nuclei up to A$\sim$60 on the basis of realistic two-nucleon (2N) interactions. However, it has become clear that three-nucleon forces (3NFs) play a major role in determining crucial features of exotic isotopes, such as the evolution of magic numbers and the position of driplines [7, 8, 9]. Realistic 2N and 3N interactions based on chiral perturbation theory have recently been evolved to low cut-offs, retaining both induced and pre-existing 3NFs [10, 11]. Proper implementations of similar hamiltonians within the above many-body theories will be required to eventually achieve quantitative predictions of medium-mass isotopes.

A second (and major) challenge to ab-initio theory is that current implementations of the above methods are limited to doubly closed (sub-)shell nuclei and their immediate neighbors [3, 6]. As one increases the nuclear mass, longer chains of truly open-shell

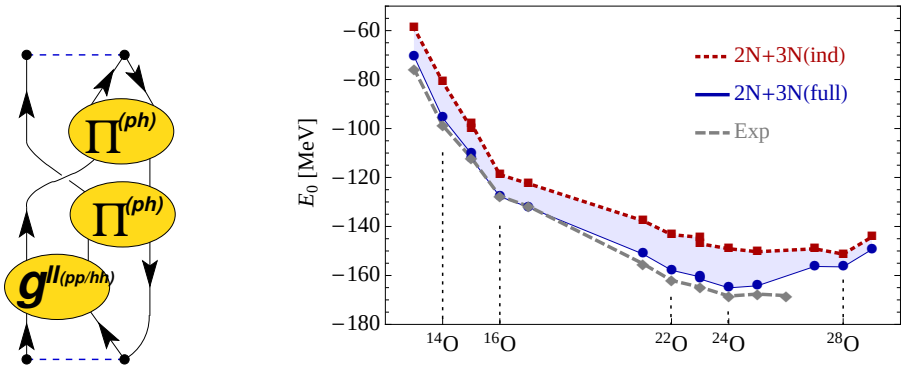

FIGURE 1. *Left:* Example of a particle-vibration coupling diagram entering the FTDA/ADC(3) self energy. *Right:* Binding energies of oxygen isotopes obtained from a SRG evolved NN+3N interactions with cutoff λ=1.88 fm^{-1}. Squares (dots) refer to induced-only (full) three-nucleon interactions and are compared to experiment (diamonds). Binding energies of even-N isotopes are obtained through the corrected Koltum sum rule (3). Odd-N energies are inferred from addition and separation energies, as obtained from the poles of the propagator (1).

nuclei connecting isolated doubly closed-shell ones emerge and cannot be accessed with existing approaches. Many-body techniques that could tackle genuine (at least) singly open-shell systems would immediately extend the reach of ab-initio studies from a few tens to several hundreds of mid-mass nuclei. A manageable way to fill this gap was recently proposed in Refs. [12, 13] by extending SCGF to Gorkov formalism and will be discussed in the following. This talk reports on recent progress on the above topics.

Three-nucleon interactions. We employ Green's function (or propagator) theory, where the object of interest is the single particle propagator [14],

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle\Psi_0^A|c_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|c_\beta^\dagger|\Psi_0^A\rangle}{\omega-(E_n^{A+1}-E_0^A)+i\eta} + \sum_k \frac{\langle\Psi_0^A|c_\beta^\dagger|\Psi_k^{A-1}\rangle\langle\Psi_k^{A-1}|c_\alpha|\Psi_0^A\rangle}{\omega-(E_0^A-E_k^{A-1})-i\eta}\,, \quad (1)$$

where $|\Psi_n^{A+1}\rangle$, $|\Psi_k^{A-1}\rangle$ are the eigenstates, and E_n^{A+1}, E_k^{A-1} the eigenenergies of the $(A\pm1)$-nucleon system. Therefore, the poles of the propagator reflect nucleon addition and separation energies. The propagator is calculated for finite closed-shell nuclei by first solving spherical Hartree-Fock (HF) equations. The HF state is then used as a reference state for the Faddeev Tamm-Dancoff (FTDA) method [a.k.a. ADC(3)] of Refs. [6]. The FTDA method completely accounts for particle-vibration diagrams as shown in Fig. 1.

We employ the intrinsic hamiltonian $H_{int} \equiv H - T_{c.m.} = \hat{U}+\hat{V}+\hat{W}$, where the kinetic energy of the center of mass has been subtracted and $\hat{U}$, $\hat{V}$ and $\hat{W}$ are the one-, two-, and three-nucleon components, respectively. Form this, we generate one- and two-nucleon density dependent interactions with matrix elements,

$$u_{\alpha\beta}^{(3NF)} = \frac{1}{2}\sum_{\gamma\sigma\mu\nu}\frac{1}{(2\pi i)^2}\int_{C\uparrow}d\omega_1\int_{C\uparrow}d\omega_2\; w_{\alpha\mu\nu,\beta\gamma\sigma}\,g_{\gamma\mu}(\omega_1)\,g_{\sigma\nu}(\omega_2)\,,$$

TABLE 1. Predicted matter radii (in fm) for ^{16}O and ^{44}Ca form SRG evolved 2N-only interactions and by including induced and full 3NF. Experiment are charge radii.

	2NF only	**2+3NF(ind.)**	**2+3NF(full)**	**Experiment**
^{16}O:	2.10	2. 41	2.38	2.718±0.210 [19]
^{44}Ca:	2.48	2.93	2.94	3.520±0.005 [20]

$$v^{(3NF)}_{\alpha\beta,\gamma\delta} \;=\; \sum_{\mu\,\nu} \frac{1}{2\pi i} \int_{C\uparrow} d\omega \;\; w_{\alpha\beta\mu,\gamma\delta\nu}\, g_{\nu\mu}(\omega)\;. \tag{2}$$

These definition extend the normal ordering approach of Ref. [11] by contracting with fully correlated propagators, as opposed to a mean-field reference state. The matrix elements $u^{(3NF)}_{\alpha\beta}$ and $v^{(3NF)}_{\alpha\beta,\gamma\delta}$ are then added to the existing 1N and 2N forces with the caveat that only interaction irreducible diagrams are retained to ensure the correct symmetry factors in the diagrammatic expansion [15].

After obtaining the sp propagator $g(\omega)$ the total binding energy can be calculated as usual through the Koltun sum rule which—due the the presence of 3NF—acquires the corrected form

$$E^A_0 = \sum_{\alpha\,\beta} \frac{1}{4\pi i} \int_{C\uparrow} d\omega \;\; \left[u_{\alpha\beta} + \omega\delta_{\alpha\beta}\right]\, g_{\beta\alpha}(\omega) \;-\; \frac{1}{2}\langle\Psi^A_0|\hat{W}|\Psi^A_0\rangle\;. \tag{3}$$

Eq. (3) is still an exact equation. However, it requires to evaluate the expectation value of the 3NF part of the hamiltonian $<\hat{W}>$ which is calculated here to first order in $\hat{W}$.

Calculations for closed sub-shell oxygen isotopes were performed for the chiral N^{3}LO 2NF [16] and N^{2}LO 3NF [17] with the cutoff of 400 MeV as introduced in Ref. [11]. These were evolved to a cutoff $\lambda = 1.88\,\mathrm{fm}^{-1}$ using free-space similarity renormalization group (SRG) [18]. We employed large model spaces of up to 12 harmonic oscillator shells with frequency $\hbar\omega$=20 MeV. Results for the induced 3NF are obtained from the SRG evolution of the original 2NF only and are indicated by red squares in Fig. 1. These are to be considered analogous to predictions of the sole N^{3}LO 2NF and systematically under bind the oxygen isotopes. Adding full 3NFs, that include in particular the two-pion exchange Fujita-Miyazawa contribution, reproduces experimental binding energies throughout the isotopic chain and the location of the neutron dripline. Table 1 shows that although SRG evolved 2NFs alone underestimate the nuclear radii, results improve with the inclusion of 3NFs.

Gorkov formalism for open-shell isotopes. The Gorkov's approach handles intrinsic degeneracies of open shell systems by allowing the breaking of particle number symmetry. One considers the grand canonical hamiltonian $\Omega_{int} = H_{int} - \mu_p\hat{Z} - \mu_n\hat{N}$ and constrains expectation values of proton and neutron number operators to the expected values. This allows defining a superfluid state which already accounts for pairing correlation and can be used as reference for Green's function diagrammatic expansion. The formalism for Gorkov self-consistent Green's function (Gorkov-SCGF) theory up to second order in the self-energy has been worked out in full in Ref. [12], for 2N interactions only. First results are reported in [13].

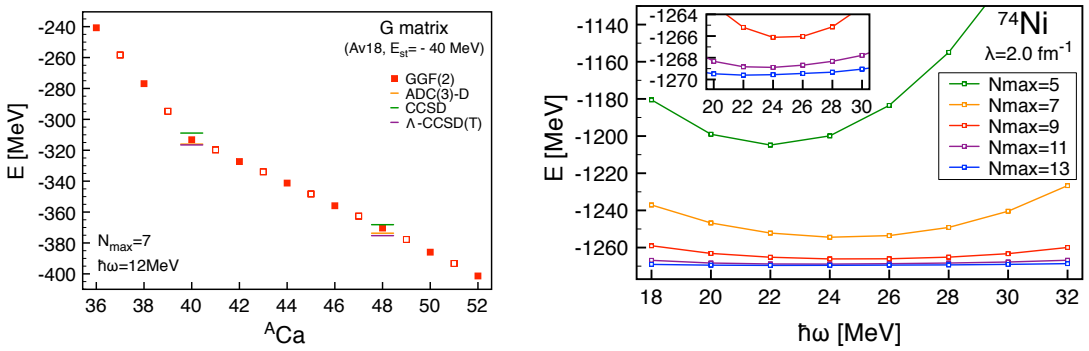

FIGURE 2. Results obtained from second-order Gorkov-SCGF *Left*: Binding energies of Ca isotopes for a fixed model space of eight shells. Gorkov propagators are calculated for even-A (filled symbols) while odd-A results (open symbols) are computed according to Ref. [21]. Closed-shell ^{40}Ca and ^{48}Ca are compared to CC and Dyson-SCGF results. *Right*: Binding energy ^{74}Ni as a function of the harmonic oscillator spacing $\hbar\omega$ and for an increasing size N_{max} of the single-particle model space.The insert shows a zoom on the most converged results.

The left panel in figure 2 displays the binding energies of calcium isotopes and compares them to single-reference CC and Dyson-SCGF for closed-shell ^{40}Ca and ^{48}Ca, using a G-matrix interaction at a fixed starting energy. Already at second-order in the self-energy, Gorkov-SCGF can provide comparable accuracy to CC singles and doubles (CCSD). Higher order corrections introduced by triples [Λ-CCSD(T)] are closely reproduced by Dyson-SCGF in the FTDA/ADC(3) approximation. Since the extension of Gorkov's formalism to ADC(3) schemes is within computational reach, this gives confidence that Gorkov-SCGF calculations can be improved to desired accuracy. The right panel displays good convergence properties, with respect to the model space, for isotopes as heavy as ^{74}Ni, using 2N SRG interactions with cutoff λ=2.0 fm^{-1}. These findings demonstrate the feasibility of first-principle calculations along full isotopic chains based on Gorkov-SCGF theory.

We further consider ^{44}Ca with the SRG, λ=2.0 fm^{-1}, interaction and add a crude estimate of 3NF by calculating the normal self-energy in a filling approximation. Full 3NFs are found to shift the neutron Fermi energy to -8.69 MeV, fairly close to the experiment. The neutron shell gap between the $0f_{7/2}$ and $0d_{3/2}$ is reduced from 12.9 MeV (2NF only) to 7.2 MeV (full 3NF). The gap between the centroids of their distributions [22] is 9.3 MeV, in agreement with data driven predictions of Ref. [23]. The calculated r.m.s. matter radius of 2.94 fm (Tab. 1) also improves with respect to 2NF only.

These are extremely encouraging results and confirm recent investigations of 3NFs [10, 11, 9]. It must be kept in mind that a correct microscopical extension to the Gorkov approach—to include missing 3NFs in both the anomalous and higher order self-energies—is still missing. This requires substantial work to develop and implement correctly the formalism and will be addressed in the coming future.

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